

Quasiparticle Nernst effect in the cuprate superconductors from the d -density wave theory of the pseudogap phase

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We consider the Nernst effect in the underdoped regime of the cuprate high temperature superconductors within the d -density wave (DDW) model of the pseudogap phase. By a combination of analytical and numerical arguments, we show that there is a robust low-temperature positive peak (*i.e.*, maximum) in the temperature dependence of the Nernst coefficient when the DDW state is ambipolar, *i.e.*, when the broken symmetry supports the coexistence of both electron- and hole-like quasiparticles in the excitation spectrum, and the electron pocket dominates at the low temperatures. In contrast, the Nernst coefficient is negative and there is no such positive peak if the underlying state is non-ambipolar, *i.e.*, when it supports only one type of quasiparticles. More generally, in the ambipolar state, the sign of the Nernst coefficient can be positive or negative depending on the dominance of the electron or hole pockets, respectively, in the low temperature thermoelectric transport. By modeling the pseudogap phase by a doping-dependent DDW order parameter with a Fermi surface topology that supports both hole and electron pockets, and assuming energy-independent transport scattering times, we analyze the evolution of the Nernst effect with doping concentration at low temperatures in the cuprate phase diagram. Even though the chosen ambipolar DDW state with a specific Fermi surface topology is not the only possible explanation of either the recent quantum oscillation experiments or the recent observation of a negative Hall coefficient at low temperatures in the underdoped cuprates, it is at least one possible state qualitatively consistent with both of these experiments. As such, the calculations in this paper present at least one possible scenario for the observed enhanced Nernst signals in the underdoped cuprates.

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I. INTRODUCTION

Even after two decades of intensive efforts, the normal state properties of the cuprate superconductors in the intermediate range of hole doping, called underdoping, are still poorly understood.¹ At low doping, close to the undoped antiferromagnetic phase,² the behavior of the system is influenced by the parent Mott insulator. At doping level above that corresponding to the maximum superconducting transition temperature (T_c), the mobile holes in the normal state constitute a Fermi liquid.³ However, at the doping range intermediate between these two limits, the system evinces a gap in the spectrum of unidentified origin (pseudogap) below a temperature scale $T^* > T_c$. Many properties of the system in this phase, called the pseudogap phase, are strongly influenced by the gap, which is, similar to the superconducting gap below T_c , anisotropic in the momentum space. An understanding of the pseudogap, and the associated loss of the spectral weight from the Fermi surface, is widely believed to hold the key to the high transition temperature in the cuprates.¹ The existence of the gap, even in the absence of super-conduction above T_c , have led many theorists to propose exotic non-Fermi-liquid states to be responsible for the pseudogap in the cuprates. However, recent quantum oscillation experiments⁴⁻⁹ have found evidence of Fermi pockets even in the enigmatic pseudogap phase. This has rekindled the

encouraging prospect of describing this phase in terms of a state with a broken symmetry and a reconstructed Fermi surface,^{5,10-15} treating its hole- and electron-like low energy quasiparticles within a well-defined Fermi-liquid-like description. Note that the Fermi arc picture, as observed in the angle resolved photoemission (ARPES) experiments,¹⁶ and the Fermi pocket picture inferred from quantum oscillation are at odds with each other, constituting a major puzzle in the field. There have been many density wave scenarios in which the coherence factors involved in ARPES, but not in quantum oscillation calculations, destroy half of the pockets, giving the appearance of a Fermi arc.^{17,18} On the other hand, ARPES has also revealed the existence of pockets in some recent experiments.^{19,20}

One of the important unsettled questions about the pseudogap phase concerns the low temperature Nernst effect. The Nernst effect experiments measure the transverse electric field response of a system to a combination set-up of an externally-imposed temperature gradient and an orthogonal magnetic field. Early experiments²¹⁻²³ on the Nernst effect in the cuprates revealed a very large signal (compared to that of a Fermi liquid) near T_c , which is expected because of the presence of the large number of mobile vortices at these temperatures. The large signal, however, appeared to onset at a temperature far above T_c , leading to speculations that there are well-defined, vortex-type, excitations even at such high temperatures. More recent experiments²⁴ have claimed

to find two peaks in the temperature dependence of the Nernst coefficient, one arising from the onset of a density wave order in the pseudogap phase, and the other due to the onset of the superconducting phase. There is also recent evidence of finding a weak peak in the Nernst signal in the pseudogap phase whose sign is opposite to that expected from the vortex-like excitations.²⁵ These recent developments, therefore, point to the importance of the quasiparticle Nernst effect associated with an underlying density wave state in the pseudogap regime of the cuprates. While the experimental scenario still needs to be settled, in this paper we deduce the full temperature and doping dependence of the quasiparticle Nernst effect associated with the d -density wave state,^{26,27} which has otherwise shown encouraging consistency with the anomalous phenomenology of the underdoped cuprates.

Since the pseudogap has a d -wave symmetry, one natural density wave state which could explain it is the $d_{x^2-y^2}$ -density wave state.^{26,27} Indeed, much of the phenomenology of the cuprates in the underdoped regime can be unified²⁷⁻²⁹ by making a single assumption that the ordered DDW state is responsible for the pseudogap. The development of the DDW order below optimal doping can lead to a consistent explanation of numerous experimental observations including the abrupt suppression of the superfluid density,³⁰ and Hall number³¹ below optimal doping as well as the more recent quantum oscillation experiments.¹⁰ Theoretically speaking, any appropriate Hamiltonian that leads to d -wave superconductivity in the underdoped regime of the cuprates will almost certainly favor DDW order as well.^{32,33} The DDW order might also have been directly observed in two polarized neutron scattering experiments,^{34,35} even though some other experiments failed to observe it.³⁶⁻³⁸ The ordered ambipolar DDW state¹⁰ and its associated Fermi surface topology (Fig. 1) are also qualitatively consistent with the quantum oscillation experiments in the pseudogap regime. The quantum oscillation experiments indicate that the Fermi surface in the underdoped cuprates is made up of small reconstructed Fermi pockets, giving rise to both hole and electron-like charge carriers (quasiparticle ambipolarity) in the excitation spectrum. Such a feature is quite robust for the DDW state, in which, for generic values of the band structure and gap parameters, the low energy spectrum consists of both electron and hole-like quasiparticles (Fig. 1).

We will derive the implications of the above important new ingredient in the cuprate physics on the quasiparticle Nernst coefficient of the DDW state. Using quasiclassical Boltzmann theory of transport, we will show that the reconstructed Fermi surface in the DDW state and its low energy quasiparticle ambipolarity can successfully explain the enhanced Nernst signals as found in the experiments at temperatures much above T_c .²¹⁻²⁴ Even though strong electronic interactions present in the host material are crucial for the formation of the DDW state,^{32,33} deep in the ordered state the quasiparticles can be assumed to be non-interacting (or weakly-interacting).

Therefore, we assume that the Boltzmann theory is still applicable to calculate the transport properties of the quasiparticles in the presence of a well-developed DDW order parameter.

By a combination of analytical and numerical arguments, we show that a low-temperature peak in the Nernst coefficient is very robust in the ambipolar d -density wave state. In fact, the existence of the peak is solely due to the dominance of the two types of quasiparticles (electron and hole) at different regimes of temperatures, and is insensitive to the microscopic details. Therefore, quasiparticle ambipolarity of the underlying state, as indicated in the quantum oscillation experiments, is also crucial for the low temperature peak in the Nernst coefficient. We also find that the sign of the peak of the Nernst effect can be positive or negative depending on the dominance of the electron or hole pockets, respectively, in the low temperature thermoelectric transport. By modeling the pseudogap by a suitable, doping-dependent, d -density wave order parameter, we analyze the doping dependent evolution of the Nernst effect at a fixed low temperature in a range of hole-concentrations in the underdoped regime of the cuprate phase diagram. The quasiparticle Nernst effect has also been recently studied³⁹ within the stripe order⁴⁰ model of the underdoped cuprates.

The paper is organized as follows: Section II introduces the commensurate DDW state and the corresponding Hartree-Fock Hamiltonian. Section III gives a brief description of the Nernst coefficient. Section IV is devoted to the temperature dependence of the Nernst coefficient. We find, both numerically and analytically, that there is a positive peak of the Nernst signal for the ambipolar DDW state when the electron pocket dominates the transport at low temperatures. In contrast, there is no such peak of the Nernst effect if the underlying state is non-ambipolar. In fact, the Nernst signal from individual electron or hole pockets are both negative, while the combination of them can lead to a positive peak. In Section V, we discuss the doping dependence of the Nernst coefficient. A positive peak in the Nernst signal as a function of hole doping is also found. Finally, we summarize and conclude in Section VI.

The main assumptions (to be explained in more detail below) we use to derive the results of this paper are: 1) Boltzmann theory is applicable to calculate the transport properties of the DDW quasiparticles, 2) The transport scattering lifetimes τ_e, τ_h (Eqs. (8, 9)) in the underdoped regime are constant over the Fermi surface and are also taken to be independent of energy in a small (temperature-dependent) interval around the Fermi energy, 3) The underlying band structure consists of both electron and hole pockets. The third assumption, that of quasiparticle ambipolarity, is the most crucial one for the qualitative robustness of the temperature and doping-dependent peaks in the DDW Nernst coefficient. Even though the existence of both types of quasiparticles as in the ambipolar DDW state is likely not the only explana-

tion of either the quantum oscillation experiments or the recent observation of negative Hall coefficients at low T in the underdoped cuprates,⁵ the ambipolar DDW state (with a specific Fermi surface topology given in Fig. (1)) is at least one possible scenario consistent with both of these experiments. As such, the Nernst calculations in this paper within the ambipolar DDW model give at least one possible explanation of the enhanced Nernst signals in the underdoped regime of the cuprates.

A part of the results (numerical calculation for the temperature dependence of the Nernst coefficient) contained in this paper were published earlier.⁴² In addition to giving a more complete discussion of these previously published results, the present paper contains the following new results: 1) An analytical explanation for the peak in the temperature dependence of the Nernst signal, 2) A fact that even though both electron and hole pockets can give negative Nernst effects individually, the combination of them can yield a positive peak as a function of temperature and 3) The full doping dependence of the DDW Nernst coefficient in the underdoped regime of the cuprates. Specifically, we show that there is a well-defined positive peak in the DDW Nernst coefficient as a function of hole doping, which is consistent with the underdoped regime in the cuprate phase diagram.

II. COMMENSURATE DDW STATE

The commensurate DDW state²⁶ is described by an order parameter which is a particle-hole singlet in spin space,

$$\langle \hat{c}_{\mathbf{k}+\mathbf{Q},\alpha}^\dagger \hat{c}_{\mathbf{k},\beta} \rangle \propto iW_{\mathbf{k}} \delta_{\alpha\beta}, \quad W_{\mathbf{k}} = \frac{W_0}{2}(\cos k_x - \cos k_y). \quad (1)$$

Here \hat{c}^\dagger and \hat{c} are the electron creation and annihilation operators on the square lattice of the copper atoms, $\mathbf{k} = (k_x, k_y)$ is the two-dimensional momentum, $\mathbf{Q} = (\pi, \pi)$ is the wave vector of the density wave, and α and β are the spin indices. For simplicity, we have taken $\hbar = 1$ and the lattice constant $a = 1$. In Eq. (1), $iW_{\mathbf{k}}$ is the DDW order parameter with the $id_{x^2-y^2}$ symmetry in the momentum space. For $\mathbf{Q} = (\pi, \pi)$, it is purely imaginary²⁶ and gives rise to spontaneous currents along the bonds of the square lattice.

The Hartree-Fock Hamiltonian describing the mean-field DDW state is given by,

$$\hat{H} = \sum_{\mathbf{k} \in \text{RBZ}} \begin{pmatrix} \varepsilon_{\mathbf{k}} - \mu & iW_{\mathbf{k}} \\ -iW_{\mathbf{k}} & \varepsilon_{\mathbf{k}+\mathbf{Q}} - \mu \end{pmatrix}, \quad (2)$$

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y, \quad (3)$$

where $\varepsilon_{\mathbf{k}}$ is the band dispersion of the electrons, and μ is the chemical potential. The Hamiltonian density in Eq. (2) operates on the two-component spinor $\hat{\Psi}_{\mathbf{k}} = (\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}+\mathbf{Q}})$ defined on the reduced Brillouin zone (RBZ) described by $k_x \pm k_y = \pm\pi$, and can be expanded over

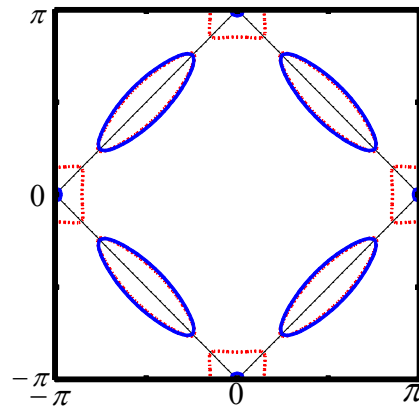


FIG. 1. (Color online) Electron and hole pockets in the ambipolar DDW state for two different chemical potentials at zero temperature. Solid (blue) lines: $\mu = -0.258$ eV ($x = 10\%$); Dashed (red) lines: $\mu = -0.238$ eV ($x = 7\%$).

the Pauli matrices $\hat{\tau}$ and the unity matrix \hat{I} ,

$$\hat{H}_{\mathbf{k}} = w_0(\mathbf{k})\hat{I} + \mathbf{w}(\mathbf{k}) \cdot \hat{\tau}, \quad w_0 = \frac{\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}+\mathbf{Q}}}{2} - \mu, \quad (4)$$

where, $w_1 = 0$, $w_2 = -W_{\mathbf{k}}$, $w_3 = \frac{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{Q}}}{2}$. The spectrum of the Hamiltonian consists of two branches with the eigenenergies given by,

$$E_{\pm}(\mathbf{k}) = w_0(\mathbf{k}) \pm w(\mathbf{k}), \quad (5)$$

where, $w(\mathbf{k}) = |\mathbf{w}(\mathbf{k})|$. For a generic set of band structure parameters, we use $t = 0.3$ eV, $t' = 0.3t$,⁴¹ and μ corresponding to a non-zero hole doping, x , appropriate for the underdoped regime of the cuprates, the reconstructed Fermi surface consists of two hole pockets near the $(\pi/2, \pm\pi/2)$ points and one electron pocket near the $(\pi, 0)$ point in the reduced Brillouin zone. The hole and the electron pockets of the DDW state are shown in Fig. 1 for two different values of the chemical potential corresponding to different values of the hole doping. The existence of both hole and electron-like excitations in the quasiparticle spectrum generically makes this state an ambipolar state.

III. NERNST COEFFICIENT

In Nernst experiments,^{21-24,43} a temperature gradient, $-\nabla T$, is applied on the sample along the \hat{x} direction. For such a temperature gradient, and with a magnetic field \mathbf{B} along the \hat{z} direction, the charge current due to quasiparticles along \hat{x} driven by $-\nabla T$ produces a balancing electric field \mathbf{E} . The total charge current in the presence of \mathbf{E} and $-\nabla T$ is thus given by,

$$J_i = \sigma_{ij} E_j + \alpha_{ij} (-\partial_j T), \quad (6)$$

where σ_{ij} and α_{ij} are the electric and the thermoelectric conductivity tensors, respectively. In the experiments, \mathbf{J}

is set to zero and the Nernst coefficient can be written as,

$$\nu_N = \frac{E_y}{(-\nabla T)_x B} = \frac{\alpha_{xy}\sigma_{xx} - \alpha_{xx}\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \quad (7)$$

where σ_{ij} and α_{ij} are the electric and the thermoelectric conductivity tensors, respectively.

For the direction of the temperature gradient as above (T decreases in the positive \hat{x} direction), and \mathbf{B} in the positive \hat{z} direction, the vortices of a superconductor produce a Nernst signal in the positive \hat{y} direction. This is because, due to entropic reasons, the vortices flow towards the cooler end. Due to the Josephson effect, the mobile vortices then produce a transverse electric field, $\mathbf{E} = \mathbf{B} \times \mathbf{v}$, which is in the positive \hat{y} direction. Note that quasiparticles in the same set up, depending on their effective charge, would produce a transverse electric field in positive or negative \hat{y} direction. Because of the uniqueness of the direction of the vortex Nernst signal,⁴³ a transverse electric field in the positive \hat{y} direction is taken as the positive Nernst signal. According to this sign convention, the Nernst coefficient of quasiparticles is positive if it is calculated to be so according to Eq. (7), where ν_N is defined in terms of E_y . This modern sign convention is opposite to the older convention sometimes also used in the literature.⁴⁴ In the Nernst experiments on the high- T_c cuprates, the modern sign convention is universally used so that the vortex signal is positive by definition.

We calculate the off-diagonal element of the conductivity tensor, σ_{xy} , by using the solution of the semi-classical Boltzmann equation:⁴⁵

$$\begin{aligned} \sigma_{xy}(\mu) = e^3 B \tau_e^2 \int \frac{d^2 k}{(2\pi)^2} & \left[\frac{\partial E_+(k)}{\partial k_x} \frac{\partial E_+(k)}{\partial k_y} \frac{\partial^2 E_+(k)}{\partial k_x \partial k_y} \right. \\ & \left. - \left(\frac{\partial E_+(k)}{\partial k_x} \right)^2 \frac{\partial^2 E_+(k)}{\partial k_y^2} \right] \left(-\frac{\partial f(E_+(k) - \mu)}{\partial E_+} \right) \\ & + (E_+ \rightarrow E_-; \tau_e \rightarrow \tau_h). \end{aligned} \quad (8)$$

Here, the momentum integrals are over the reduced Brillouin zone. In the DDW band-structure, the electron pocket near $(\pi, 0)$ is associated with the upper band, $E_+(\mathbf{k})$. The first integral in Eq. (8), therefore, embodies the contribution to σ_{xy} due to the electron-like quasiparticles. We have denoted the corresponding transport scattering time as τ_e , which, for simplicity, is taken to be independent of the location on the electron Fermi line. The second integral in Eq. (8), where τ_e is replaced by the scattering time for the hole-like careers, τ_h , calculates the contribution to σ_{xy} from the hole pockets. τ_h is also taken to be constant everywhere on the hole Fermi lines. Even though both the scattering times can be energy-dependent,⁴⁶ since the Fermi surface integrals in Eq. (8) and Eq. (9) (see below) extend only over a small (temperature-dependent) interval around the Fermi energy, we assume τ_e and τ_h to be energy independent in our calculations.

In general, there is no obvious reason to expect $\tau_e = \tau_h$. For a consistent interpretation of the Hall effect experiments,⁵ it has been recently argued that the scattering times, which are directly proportional to the career mobilities, may in fact be different for the electron and the hole-like charge carriers. Since at low temperatures the Hall coefficient is negative, Ref. [5] argues that, at least at low T , $\tau_e > \tau_h$. With the above definition of the parameters, the diagonal element of the conductivity tensor is given by,⁴⁵

$$\begin{aligned} \sigma_{xx}(\mu) = e^2 \tau_e \int \frac{d^2 k}{(2\pi)^2} & \left(\frac{\partial E_+(k)}{\partial k_x} \right)^2 \left(-\frac{\partial f(E_+(k) - \mu)}{\partial E_+} \right) \\ & + (E_+ \rightarrow E_-; \tau_e \rightarrow \tau_h). \end{aligned} \quad (9)$$

From the solution of the Boltzmann equation at low T , the thermoelectric tensor α_{ij} is related to the conductivity tensor σ_{ij} by the Mott relation:⁴⁷

$$\alpha_{ij} = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{\partial \sigma_{ij}}{\partial \mu}. \quad (10)$$

Here $e > 0$ is the absolute magnitude of the charge of an electron. Using Eq. (7), the formula for the Nernst coefficient reduces to,⁴⁸

$$\nu_N = -\frac{\pi^2}{3} \frac{k_B^2 T}{e B} \frac{\partial \Theta_H}{\partial \mu} \quad (11)$$

Here,

$$\Theta_H = \tan^{-1} \left(\frac{\sigma_{xy}}{\sigma_{xx}} \right). \quad (12)$$

Using Eqs. (8,9,11) and with reasonable phenomenological assumptions about the temperature dependence of the scattering times and the DDW order parameter, we can now calculate ν_N as a function of T in the ambipolar DDW state. Using a phenomenological ansatz for the doping dependence of the DDW order parameter, and computing the chemical potential self-consistently, we can also use the same equations to calculate the doping dependence of ν_N . This way we can evaluate the evolution of the Nernst coefficient in the cuprate phase diagram within the ambipolar DDW model.

It is important to emphasize that the negative Hall coefficient at low T , as seen in the presence of strong magnetic fields in Ref. [5], does not automatically imply the presence of the electron pockets at low enough magnetic fields. However, conversely, the existence of the electron pockets in the band-structure is at least one possible scenario consistent with the negative Hall coefficient. In addition, the existence of the electron pockets is also qualitatively consistent with the observed frequencies in the recent quantum oscillation experiments. Our calculated enhanced Nernst coefficients are for the ambipolar DDW state which has both electron- and hole-like quasiparticles in the excitation spectrum. As such, the results of this paper give at least one possible explanation of the observed enhanced Nernst signals in the underdoped cuprates.

IV. TEMPERATURE DEPENDENCE OF THE NERNST COEFFICIENT

A. Phenomenological temperature dependence of the parameters

In the first step in the evaluation of the temperature dependence of the Nernst coefficient, we have to make suitable assumptions for the behavior of the scattering times τ_e and τ_h with temperature. An important hint regarding this can be obtained from the recent Hall effect experiments in Ref. 5. In these experiments, the normal state Hall coefficient,

$$R_H = \frac{\sigma_{xy}}{B(\sigma_{xx})^2}, \quad (13)$$

has been measured as a function of T in three different samples of underdoped YBCO. In all three samples, R_H is large and positive above T^* , which is consistent with the systems being moderately hole doped. R_H , however, shows a sharp decline below T^* , and subsequently changes its sign from positive (hole-dominated) to negative (electron-dominated) at a crossover temperature $T_0 < T^*$. This anomalous T -dependence of the Hall coefficient can be understood naturally if the state in question below T^* is inherently ambipolar, and the mobilities of the oppositely charged quasiparticles are assumed to be unequal and changing with temperature.

With Eqs. (8,9), we can calculate the contributions of the electron and hole pockets of the DDW state to the normal state Hall coefficient. The magnitudes of the individual contributions depend on the size and curvature of the respective pockets, but in our calculations the sign of the contribution is positive for the hole-like quasiparticles and negative for the electron-like quasiparticles. For $\tau_e = \tau_h$, in which case the formula for R_H is independent of the scattering time, and for a generic set of parameters (t, t', W_0) consistent with the quantum oscillation experiments in YBCO,^{10,17} the size and curvature of the hole pockets are much bigger than those of the electron pocket. This implies that, for $\tau_e \sim \tau_h$, the sign of the overall R_H is positive.³¹ We have checked that reasonable modifications of the band structure parameters in the cuprate phase diagram cannot change this result. Therefore, within the Boltzmann theory of transport, the only source of the strong T -dependence of R_H , as observed in the experiments, must come from the unequal temperature dependence of τ_e and τ_h . If at high temperatures ($T > T_0$) $\tau_e \sim \tau_h$, the Hall coefficient is positive. On the other hand, if $\tau_e > \tau_h$ for $T < T_0$, R_H can become negative at low T . Note that a higher mobility of the electron-like quasiparticles at low T is also consistent with the frequency observed in the quantum oscillation experiments.^{5,10} An independent, microscopic, justification of the higher lifetime of the electron-like quasiparticles at low T and in the presence of a magnetic field also follows by considering the scattering of both types of quasiparticles by vortices at low temperatures.⁴⁹ Be-

cause of the difference of the effective masses between the DDW quasiparticles near the antinodal and the nodal regions in the Brillouin zone, the electron lifetime due to vortex scattering can be significantly higher than the hole lifetime at low T in the presence of a magnetic field.⁵⁰

On the above grounds, we choose the minimal T -dependence of the scattering times:

$$\hbar\tau_e^{-1} = A_e + B_e k_B T \quad (14)$$

and

$$\hbar\tau_h^{-1} = A_h + B_h k_B T \quad (15)$$

Even though such a linear T -dependence of the scattering times is nominally consistent with the linear T -dependence of the resistivity in a regime close to the optimal doping in the cuprate phase diagram, we emphasize that our motivation for the assumptions about τ_e and τ_h is strictly phenomenological. With these choices, the calculated $R_H = \frac{\sigma_{xy}}{B\sigma_{xx}^2}$ for the ambipolar DDW state as a function of T with an assumed mean field T -dependence of the DDW order parameter,

$$W_0(T) = W_0 \sqrt{1 - \frac{T}{T^*}} \quad (16)$$

($T^* \sim 110$ K), qualitatively agrees with the recent experiments.⁵ We estimate the values of the temperature independent parameters A_e, B_e, A_h, B_h in Eq. (14) and Eq. (15) from the qualitative agreement of the Hall effect experiments in the underdoped cuprates. We do this by setting the total R_H to zero at $T = T_0 = 30$ K. This provides one equation relating the four unknown constants. Then we assume that at high temperatures τ_e approximately equals τ_h , which stipulates $B_e \sim B_h$. We take them both to be equal to 1 for simplicity. Therefore, we are left with two unknowns A_e and A_h and only one equation relating them, which leaves some residual freedom in choosing the values of these constants. However, we have checked that our conclusions for the behavior of ν with T are robust to any reasonable variation of the T -dependence of τ_e, τ_h and $W_0(T)$ as long as they satisfy the experimental constraints set by the temperature dependence of R_H .

We now use Eqs. (8, 9, 11) to calculate ν_N as a function of T for a specific value of the hole doping $x = 10\%$. Using a mean field T -dependence of $W_0(T)$ and the phenomenological form of $\tau_e(T)$ and $\tau_h(T)$ above, we plot in Fig. (2) the calculated ν_N in the ambipolar DDW state as a function of T for $x = 10\%$. It is clear from Fig. (2) that the Nernst coefficient has a pronounced low temperature peak which, as we argue below, is a direct manifestation of the quasiparticle ambipolarity of the DDW state.

B. Sign and temperature dependence of Nernst signal from individual hole and electron pockets

To elucidate the importance of the quasiparticle ambipolarity in the temperature dependence of ν_N , let us

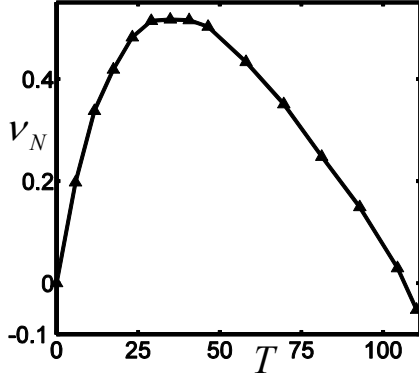


FIG. 2. Plot of the Nernst coefficient, ν_N , versus temperature T for the ambipolar DDW state. The Nernst coefficient in $\text{V K}^{-1}\text{T}^{-1}$ can be derived by multiplying the dimensionless ν_N in the figure with the quantity $2\pi^2 k_B a^2 / 3\hbar \approx 138 \text{ nV/KT}$. Here the lattice constant is taken as $a \sim 0.4 \text{ nm}$, and the factor 2 is used to account for the contributions from the two spin components. The peak value is $\sim 70 \text{ nV/KT}$ at a temperature $T < T^*$. The unit for T along the horizontal axis is K . The hole doping $x = 10\%$. The sign of ν_N near its peak is positive. As the superconducting T_c (not shown here) is approached, the normal state ν_N as shown here will be cut-off by the large Nernst signal of the mobile vortices associated with the superconductor. The parameters used in the plot are $T^* = 110 \text{ K}$, $A_e/k_B = 58 \text{ K}$, $A_h/k_B = 253 \text{ K}$, $t = 0.3 \text{ eV}$, $t' = 0.3t$, $B_e = B_h = 1$, $W_0 = 0.1 \text{ eV}$, $\mu = -0.258 \text{ eV}$.

first consider the Nernst effect due to the quasiparticles associated with a hole pocket. In the presence of only hole pockets in the excitation spectrum, we can write the Nernst coefficient as

$$\nu_N^h = -C\tau_h T \frac{\partial}{\partial \mu} \bar{\Theta}^h, \quad (17)$$

where we take

$$\bar{\Theta}^h \approx \frac{\bar{\sigma}_{xy}^h}{\bar{\sigma}_{xx}^h}, \quad (\bar{\sigma}_{xy}^h \ll \bar{\sigma}_{xx}^h) \quad (18)$$

$$\bar{\sigma}_{xy}^h = \sigma_{xy}^h / \tau_h^2, \quad \bar{\sigma}_{xx}^h = \sigma_{xx}^h / \tau_h \quad (19)$$

and C is a numerical constant, $C = \frac{\pi^2 k_B^2}{3 e B}$. $\bar{\sigma}_{xy}^h$ and $\bar{\sigma}_{xx}^h$ (superscript h indicates the contribution from the hole-like quasiparticles) depend only on the hole Fermi surface integrals in Eq. (8) and Eq. (9), respectively. We have rewritten the expression for ν_N (Eq. (11)) in Eq. (17) so that the manipulation of the explicit T -dependence of the scattering time becomes easier. Similarly, when there are only electron-like quasiparticles in the system, the Nernst coefficient can be written as,

$$\nu_N^e = -C\tau_e T \frac{\partial}{\partial \mu} \bar{\Theta}^e, \quad (20)$$

where $\bar{\Theta}^e \approx \frac{\bar{\sigma}_{xy}^e}{\bar{\sigma}_{xx}^e}$, $\bar{\sigma}_{xy}^e = \sigma_{xy}^e / \tau_e^2$, $\bar{\sigma}_{xx}^e = \sigma_{xx}^e / \tau_e$, and the superscript e indicates electron-like quasiparticles.

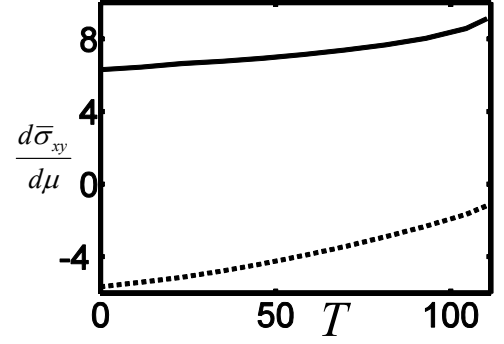


FIG. 3. Plot of $\frac{d\bar{\sigma}_{xy}}{d\mu}$ versus temperature for the electron and hole pockets using Eqs. (8,19). The unit of T is K , and the unit for $\frac{d\bar{\sigma}_{xy}}{d\mu}$ is unimportant for the purpose of this illustration. $x = 10\%$. Dashed line: electron; Solid line: hole.

In the following analysis, we will frequently need the sign of the quantities, $\frac{d\bar{\sigma}_{xy}^h}{d\mu}$, $\frac{d\bar{\sigma}_{xx}^h}{d\mu}$, and their counterparts for the electron pockets. These can be deduced by noting the changes in the shapes of the hole and the electron pockets with increasing μ (μ becoming less negative). To do this, we recall that the magnitude of $\bar{\sigma}_{xy}$ increases with the curvature of the relevant pocket, and the magnitude of $\bar{\sigma}_{xx}$ increases with its area. In Fig. 1, we plot the electron and hole pockets for two different values of the chemical potential. As we can see, as μ increases, the hole pockets become more elliptical (i.e., the curvature rises and the circumference decreases), thus $\frac{d\bar{\sigma}_{xy}^h}{d\mu} > 0$ and $\frac{d\bar{\sigma}_{xx}^h}{d\mu} < 0$. On the other hand, for the electron pocket, the size of the pocket increases with increasing μ , leading to $\frac{d\bar{\sigma}_{xx}^e}{d\mu} > 0$. It is not clear, however, how the curvature of the electron pocket varies with μ . In Fig. (3), we plot the $\frac{d\bar{\sigma}_{xy}^e}{d\mu}$ and $\frac{d\bar{\sigma}_{xx}^h}{d\mu}$ for $x = 10\%$. We clearly see that $\frac{d\bar{\sigma}_{xy}^e}{d\mu} < 0$ and $\frac{d\bar{\sigma}_{xx}^h}{d\mu} > 0$. For the hole pockets, the above behaviors lead to

$$\frac{\partial \bar{\Theta}^h}{\partial \mu} = \frac{1}{(\bar{\sigma}_{xx}^h)^2} \left(\frac{d\bar{\sigma}_{xy}^h}{d\mu} \bar{\sigma}_{xx}^h - \frac{d\bar{\sigma}_{xx}^h}{d\mu} \bar{\sigma}_{xy}^h \right) > 0. \quad (21)$$

This implies that the hole pockets lead to a negative Nernst signal, as seen from Fig. 4. The analysis of the sign of the Nernst coefficient from the electron pocket is not so straightforward, and will be discussed later.

Taking the temperature derivative of ν_N^h in Eq. (17), we get,

$$\begin{aligned} C^{-1} \frac{\partial \nu_N^h}{\partial T} &= -\tau_h \frac{\partial \bar{\Theta}^h}{\partial \mu} - T \frac{\partial \tau_h}{\partial T} \frac{\partial \bar{\Theta}^h}{\partial \mu} - T \tau_h \frac{\partial}{\partial T} \frac{\partial \bar{\Theta}^h}{\partial \mu} \\ &= -\frac{1}{T + A_h} \left(1 - \frac{T}{T + A_h} \right) \frac{\partial \bar{\Theta}^h}{\partial \mu} \\ &\quad - T \tau_h \frac{\partial}{\partial T} \frac{\partial \bar{\Theta}^h}{\partial \mu}, \end{aligned} \quad (22)$$

where we take $B_h = 1$. In Eq. (22), the first term on the

right hand side is the result of the explicit T -dependence of ν_N via the scattering time and the explicit factor of T . Since $\frac{\partial \bar{\Theta}^h}{\partial \mu}$ is positive, this term is strictly negative. The second term in Eq. (22) depends on the implicit T -dependence of ν_N^h via the T -dependence of W_0 . To calculate this term, we write,

$$\frac{\partial}{\partial T} \frac{\partial \bar{\Theta}^h}{\partial \mu} = \frac{\partial}{\partial \mu} \frac{\partial \bar{\Theta}^h}{\partial T} = \frac{\partial}{\partial \mu} \left(\frac{\partial \bar{\Theta}^h}{\partial W_0} \frac{-1}{2(T^* - T)^{1/2}} \right), \quad (23)$$

where we have used the mean field ansatz for the T -dependence of the amplitude of the DDW order parameter. To calculate the right hand side, noting that T is independent of μ , we only need to calculate,

$$\begin{aligned} \frac{\partial}{\partial \mu} \frac{\partial \bar{\Theta}^h}{\partial W_0} &= \frac{\partial}{\partial \mu} \frac{1}{\bar{\sigma}_{xx}^h} \left(\frac{d\bar{\sigma}_{xy}^h}{dW_0} - \bar{\Theta}^h \frac{d\bar{\sigma}_{xx}^h}{dW_0} \right) \\ &\approx -\frac{1}{(\bar{\sigma}_{xx}^h)^2} \frac{\partial \bar{\sigma}_{xx}^h}{\partial \mu} \left(\frac{d\bar{\sigma}_{xy}^h}{dW_0} - \bar{\Theta}^h \frac{d\bar{\sigma}_{xx}^h}{dW_0} \right) \\ &\quad - \frac{1}{\bar{\sigma}_{xx}^h} \frac{\partial \bar{\Theta}^h}{\partial \mu} \frac{d\bar{\sigma}_{xx}^h}{dW_0}. \end{aligned} \quad (24)$$

In the derivation of the above equation, we neglect the small terms $\frac{\partial}{\partial \mu} \frac{d\bar{\sigma}_{xy}^h}{dW_0}$ and $\frac{\partial}{\partial \mu} \frac{d\bar{\sigma}_{xx}^h}{dW_0}$ (see Eq. (25) below for justification). It is clear that we first need the leading W_0 -dependence of the Fermi surface integrals $\bar{\sigma}_{xy}^h$ and $\bar{\sigma}_{xx}^h$. We find that the leading W_0 dependence of these integrals is linear. This linear dependence arises from the integration region around the so-called *hot spots*, points on the Fermi surface which also fall on the surface of the RBZ. On the surface of the RBZ ($k_x \pm k_y = \pm\pi$), the dominant part of the band structure, $-2t(\cos k_x + \cos k_y) = 0$. The linear W_0 dependence of $\bar{\sigma}_{xy}^h$ and $\bar{\sigma}_{xx}^h$ comes from the

region around the hot spots which satisfies

$$t|\cos k_x + \cos k_y| < \frac{W_0}{4} |\cos k_x - \cos k_y|,$$

which has a size $\sim tW_0$. Since the relevant integration region is itself $\mathcal{O}(W_0)$, by expanding the integrand in Eq. (8) to zeroth order in W_0 , we get the leading W_0 dependence of $\bar{\sigma}_{xy}^h$ as,

$$\bar{\sigma}_{xy}^h \sim 64tW_0 t'^3 \sin^2 k_x \cos k_x \cos k_y. \quad (25)$$

The above is negative since $\cos k_x = -\cos k_y$ on the surface of RBZ. Therefore, it follows that, $\frac{d\bar{\sigma}_{xy}^h}{dW_0} < 0$. From similar manipulations, it is straightforward to show that $\frac{d\bar{\sigma}_{xx}^h}{dW_0} > 0$. We also note that, in Eq. (24), $\bar{\Theta}^h$ itself is positive for the hole pockets ($\bar{\Theta}^h$ has the same sign as the Fermi surface integral for the Hall conductivity, $\bar{\sigma}_{xy}^h$, which is, of course, positive for the hole pockets). Furthermore, noting that $\frac{\partial \bar{\sigma}_{xx}^h}{\partial \mu} < 0$ and $\frac{\partial \bar{\Theta}^h}{\partial \mu} > 0$ for the hole pocket, we infer from Eq. (24) that $\frac{\partial}{\partial \mu} \frac{\partial \bar{\Theta}^h}{\partial W_0} < 0$. Therefore, from Eq. (23),

$$\frac{\partial}{\partial T} \frac{\partial \bar{\Theta}^h}{\partial \mu} = \frac{\partial}{\partial \mu} \frac{\partial \bar{\Theta}^h}{\partial T} > 0 \quad (26)$$

for $T < T^*$. Finally, using Eq. (22), we conclude that $\frac{\partial \nu_N^h}{\partial T}$ is negative definite for the hole pockets. This implies that, for only hole-type quasiparticles in the DDW state, the temperature-derivative of the Nernst coefficient can never be zero: there is no low temperature peak of $\nu_N^h(T)$. This analytical result has been confirmed by the numerical results, as seen in Fig. 4.

In contrast to ν_N^h , the sign of ν_N^e is hard to determine analytically. The reason is that, in

$$\frac{\partial \bar{\Theta}^e}{\partial \mu} = \frac{1}{(\bar{\sigma}_{xx}^e)^2} \left(\frac{d\bar{\sigma}_{xy}^e}{d\mu} \bar{\sigma}_{xx}^e - \frac{d\bar{\sigma}_{xx}^e}{d\mu} \bar{\sigma}_{xy}^e \right),$$

the terms $\frac{d\bar{\sigma}_{xy}^e}{d\mu} \bar{\sigma}_{xx}^e (< 0)$ and $-\frac{d\bar{\sigma}_{xx}^e}{d\mu} \bar{\sigma}_{xy}^e (> 0)$ have opposite signs, and the sign of ν_N^e should be determined by the relative magnitudes of these two terms. For the band structure parameters used here, we find that ν_N^e is negative, as seen in Fig. 4. This implies that, for the electron pocket, the second term in $\frac{\partial \bar{\Theta}^e}{\partial \mu}$ dominates over the first one, leading to a positive $\frac{\partial \bar{\Theta}^e}{\partial \mu}$.

C. Temperature dependence of the Nernst coefficient from ambipolar DDW state

In view of the above analysis, a natural question is then why two individually negative contributions from the electron and the hole pockets ‘add up’ to a positive Nernst signal at low temperatures when the two types of pockets coexist. The underlying reason can be most

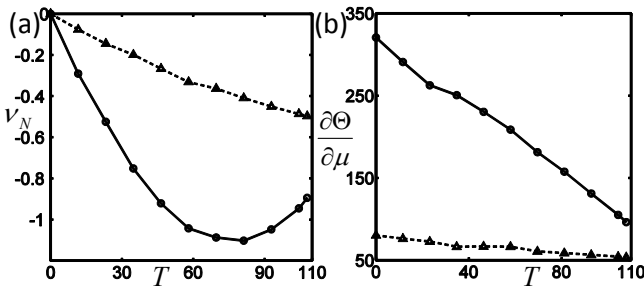


FIG. 4. (a) Plot of the Nernst coefficient, ν_N , versus temperature for the electron (solid line) and hole (dashed line) pockets separately. The parameters used in the plot are same as those in Fig. 2. Nernst coefficient in $\text{V K}^{-1}\text{T}^{-1}$ can be derived by multiplying the dimensionless ν_N in the figure with the factor $2\pi^2 k_B a^2 / 3\hbar \approx 138 \text{ nV/KT}$. The temperature in the horizontal axis is in K . The hole doping $x = 10\%$. (b) Plots of $\frac{\partial \nu_N}{\partial T}$ versus temperature for the electron and hole pockets separately. The plots in (a) are obtained by multiplying these values by $-k_B T$ in eV .

clearly expressed by writing down the formula for $\frac{\partial \Theta^t}{\partial \mu}$, where the superscript ‘t’ now represents the total Nernst effect as given by multiplying $\frac{\partial \Theta^t}{\partial \mu}$ by $-CT$,

$$\frac{\partial \Theta^t}{\partial \mu} = \frac{1}{(\sigma_{xx}^t)^2} \left(\frac{d\sigma_{xy}^t}{d\mu} \sigma_{xx}^t - \frac{d\sigma_{xx}^t}{d\mu} \sigma_{xy}^t \right) \quad (27)$$

Here, $\sigma_{xx}^t = \sigma_{xx}^h + \sigma_{xx}^e$ and $\sigma_{xy}^t = \sigma_{xy}^h + \sigma_{xy}^e$. Because of the ambipolar spectrum, the second term in Eq. (27) is much smaller than the first one (since the total Hall conductivity, σ_{xy}^t , is small), and the sign of $\frac{\partial \Theta^t}{\partial \mu}$ is entirely determined by the first term. It follows that if the contribution from the electron pocket dominates over that from the hole pocket, then $\frac{\partial \Theta^t}{\partial \mu}$ is negative, since the first term in Eq. (27) is negative for the electron pocket. On the other hand, if the contribution from the hole pocket is greater than that from the electron pocket, then $\frac{\partial \Theta^t}{\partial \mu}$ is positive because $\frac{d\sigma_{xy}^h}{d\mu}$ is positive for the hole pocket, see Fig. 3. In our calculations, the former is the situation at low T , and ν_N is positive at low temperatures. At high temperatures, the contribution from the hole pockets dominates transport because of their larger size and the first term in Eq. (27), and consequently $\frac{\partial \Theta^t}{\partial \mu}$, becomes positive, leading to a negative Nernst signal. Therefore, ν_N , which is zero at $T = 0$, first increases at low temperatures and then decreases at high temperatures, yielding a positive peak if there are both electron- and hole-type quasiparticles present in the spectrum at the same time.

In the context of the cuprates, at low temperatures, the electron pocket dominates via $\tau_e \gg \tau_h$, and $\frac{\partial \nu_N}{\partial T} > 0$. On the other hand, at high temperatures, the hole pockets dominate when $\tau_e \sim \tau_h$. In this case, we have $\frac{\partial \nu_N}{\partial T} < 0$. In practice, determining an analytical expression for the peak temperature by solving the implicit equation, $\frac{\partial \nu_N}{\partial T} = 0$, is not very illuminating, since it depends on many parameters. However, we have conclusively shown here that the existence of a low temperature positive peak in the Nernst coefficient is a robust consequence of quasiparticle ambipolarity, and, therefore, is independent of any assumptions about the microscopic parameters. Furthermore, the sign of the peak value of $\nu_N(T)$ depends on the relative dominance of the electron and the hole pockets at different regimes of T . For example, if the hole (electron) pockets were dominant at low (high) temperatures, the peak value of $\nu_N(T)$ would be negative. However, in the experimentally relevant case where the electron pocket is more dominant at low T (so that the zero temperature Hall coefficient is negative), the peak is on the positive side.

V. DOPING DEPENDENCE OF THE NERNST COEFFICIENT

To calculate the Nernst coefficient as a function of doping in the underdoped regime, we have to start by assuming a phenomenological doping dependence of the DDW

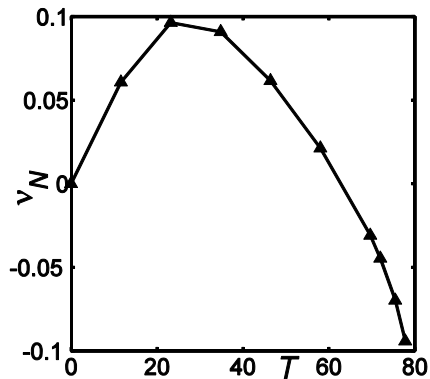


FIG. 5. The Nernst coefficient as a function of temperature for $x = 7\%$. Nernst coefficient in $\text{V K}^{-1}\text{T}^{-1}$ can be derived by multiplying ν_N with the factor $2\pi^2 k_B a^2 / 3\hbar \approx 138 \text{ nV/KT}$. The temperature is in K. The corresponding $\mu = -0.238 \text{ eV}$, $T^* = 80 \text{ K}$. We see that the Nernst signal is negative in a broader temperature regime than that for $x = 10\%$.

order parameter W_0 . Using the values of the doping-dependent amplitude of the DDW order parameter and the set of parameters t, t', x , we can calculate the chemical potential μ as a function of x . This way, the Nernst coefficient can be calculated as a function of the doping in the pseudogap phase. In the absence of a concrete theoretical result for the doping dependence of the DDW order parameter, we assume the mean-field doping dependence,

$$W_0(x, T) = W_0(x_0, T) \begin{cases} \sqrt{\frac{x_{\max} - x}{x_{\max} - x_0}} & \text{if } x \geq x_0 \\ \sqrt{\frac{x - x_{\min}}{x_0 - x_{\min}}} & \text{if } x < x_0 \end{cases} \quad (28)$$

where $x_0 = 10\%$ is the doping percentage that yields the maximum DDW order. This kind of a doping dependence is physically motivated, since we expect the DDW order to gradually weaken for both high and low values of x . We choose $x_{\min} = 4\%$ and $x_{\max} = 17\%$ as the minimum and the maximum doping where the DDW order may exist. We use the value of x and the set of parameters $t, t', W_0(x, T = 0)$ to self-consistently calculate the value of μ , which determines the size and curvature of the hole and the electron pockets.

To illustrate the behavior of ν_N with underdoping, we plot in Fig. (5) the temperature dependence of ν_N for $x = 7\%$. It is clear that the Nernst signal remains negative in a wider range of temperatures at this value of hole-doping than that at $x = 10\%$. However, there is still a small low temperature peak in the positive side because of the larger mobility of the electron pocket at low temperatures. Since the Nernst effect at temperatures close to and below the superconducting T_c is almost entirely dominated by the vortex Nernst signal, the low temperature positive peak due to the DDW quasiparticles may not be visible in the experiments. In this case, the DDW quasiparticle Nernst effect may appear negative above the superconducting T_c .

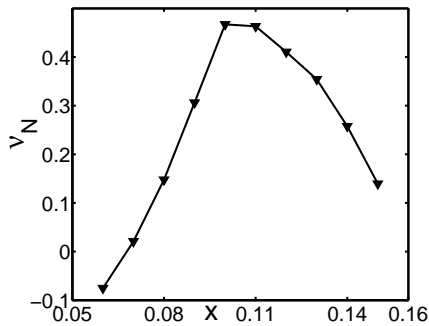


FIG. 6. Plot of the Nernst coefficient, ν_N , at a fixed low temperature, $T = 58$ K, versus the hole doping x for the ambipolar DDW state. Nernst coefficient in $\text{V K}^{-1}\text{T}^{-1}$ can be derived by multiplying ν_N with the factor $2\pi^2 k_B a^2 / 3\hbar \approx 138$ nV/KT. The temperature is in K. Nernst coefficient shows a pronounced peak at a hole doping $x = 10\%$, where the DDW order parameter is assumed to be the largest. The sign of ν_N near its peak is positive.

In Fig. (6), we plot the Nernst coefficient at a fixed low temperature as a function of hole doping x . To construct this plot, we have taken the transition temperature of the ordered DDW state to scale with the value of the zero temperature order parameter, as would be expected from the mean field theory. This implies that $T^*(x)$ has been determined via

$$T^*(x) = \frac{W_0(x, T=0)}{W_0(x_0, T=0)} T^*(x_0). \quad (29)$$

It is clear that there is a peak of the Nernst signal at $x = 10\%$ on the positive side, in agreement with the Nernst effect experiments^{21–23} in the cuprates. The signal weakens on either side of $x = 10\%$ because the magnitude of the DDW order parameter weakens with x on either side of this value of doping.

VI. CONCLUSION

In conclusion, we show that the Nernst signal from an ambipolar DDW state has a robust low temperature peak which occurs below its mean field transition temperature. The onset of the Nernst signal, however, occurs at the transition temperature itself, which may account for the sizable Nernst effect found in the experiments in the pseudogap phase of the high temperature cuprate superconductors. The sign of the peak value of the Nernst coefficient can be positive or negative depending on whether electron- or hole-pockets, respectively, dominate the low

temperature thermoelectric transport. For the experimental situation in some cuprates, where the low temperature Hall coefficient is found to be negative indicating the dominance of the electron pocket in transport, we find that the peak in the temperature dependent Nernst coefficient is on the positive side. In contrast, there is no such peak when the DDW state is non-ambipolar. In this case, with only one type of pockets in the excitation spectrum, the Nernst signal is negative for both electron and hole pockets. However, quite surprisingly, we find that these two individual negative contributions ‘add up’ to produce a net positive Nernst effect in the ambipolar DDW state. We prove these results both by numerical calculations as well as analytical arguments, which establishes the robustness of the existence of the low temperature peak, making it insensitive to any reasonable variations of the microscopic parameters.

With a reasonable assumption about the doping dependence of the DDW order parameter, which is physically motivated and stipulates weakening of the order parameter with hole doping on either side of the underdoped regime, we find that the low temperature Nernst coefficient also has a pronounced peak as a function of hole concentration. The peak of the Nernst coefficient coincides with the value of doping where the DDW order parameter is assumed to be the strongest, and the signal weakens on either side of this value of the hole concentration. At low value of the hole doping, we find that the Nernst coefficient remains negative over a wider range of temperature than at moderate underdoping, $x = 10\%$.

To derive these results, we model the pseudogap phase by a doping-dependent DDW order parameter and assume transport scattering times which are constant throughout the Fermi surface and also independent of energy in a small (T -dependent) energy interval around the Fermi energy. Even though our chosen ambipolar DDW state (with its specific Fermi surface topology (Fig. (1)) is not the only possible state consistent with either the recent quantum oscillation experiments^{4–9} or the observed negative Hall coefficient⁵ in the underdoped cuprates, it is at least one possible state qualitatively consistent with both. As such, the calculations for the Nernst coefficient in the ambipolar DDW state given in this paper present at least one possible scenario for the observed enhanced Nernst signals in the underdoped cuprate superconductors.

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